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Solution of periodic Poisson's equation and the Hartree-Fock approach for solids with extended electron states: application to linear augmented plane wave method

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We would like to notice that the issue of the Hartree-Fock LAPW (linear augmented plane wave) approach was considered before by S. Massidda, M. Posternak, and A. Baldereschi in Phys. Rev. B **48**, pp. 5058-5068 (1993), but we were unaware of this publication. We thank D.J. Singh and M. Weinert for this reference.

Eq. (2.5a) is missing the contributions from $\vec{K} \neq 0$, i.e. it should read as

$$\begin{aligned} \rho'_0(r) = & \rho_0(r) - \sqrt{4\pi}\rho_I(\vec{K}=0) - Z \frac{\delta(r)}{\sqrt{4\pi}r^2} \\ & - \sqrt{4\pi} \sum'_{\vec{K} \neq 0} j_0(Kr) \rho_I(\vec{K}). \end{aligned} \quad (2.5a)$$

Correspondingly, Eqs. (2.11) acquire additional terms:

$$\begin{aligned} Q_0(r) = & q_0(r) - \frac{4\pi r^3}{3} \rho_I(\vec{K}=0) \\ & - 4\pi r^2 \sum'_{\vec{K} \neq 0} \frac{j_1(Kr)}{K} \rho_I(\vec{K}), \end{aligned} \quad (2.11a)$$

$$\begin{aligned} Q'_0(r) = & q'_0(r) - 2\pi(R^2 - r^2) \rho_I(\vec{K}=0) \\ & + 4\pi \sum'_{\vec{K} \neq 0} (\cos(KR) - \cos(Kr)) \frac{\rho_I(\vec{K})}{K^2}. \end{aligned} \quad (2.11b)$$

The additional terms are the last ones in Eq. (2.5a),

Eq. (2.11a) and Eq. (2.11b).

For the cases which we consider in Sec. 3 though this does not make any difference.

Eq. (3.3) should read as

$$E_{fcc}/N = \frac{1}{2} (V_0^{out} - \langle V_I \rangle) = -1.2079 \text{ a.u.} \quad (3.3)$$

More details on the Madelung potential are given by M. Weinert, E. Wimmer, and A.J. Freeman in Phys. Rev. B **26**, 4571 (1982).

We thank M. Weinert for these corrections and for discussing the results of our work.

Finally, for clarity we would like to notice that the exact solutions $V_{04}(exact)$ and $V_{06}(exact)$ in Figures 2 and 3 are given explicitly by

$$\begin{aligned} V_{04}^{(exact)}(r) &= \tilde{V}_{04} \left(\frac{r}{R} \right)^4, \\ V_{06}^{(exact)}(r) &= \tilde{V}_{06} \left(\frac{r}{R} \right)^6. \end{aligned}$$

Here $\tilde{V}_{04} = -0.18192$, $\tilde{V}_{06} = -0.14466$ are exact values at the radius $R = \sqrt{2}/4$ (see last row of Table II). Thus, in Figures 2 and 3 we depict the deviations from those exact dependences for two solutions (Weinert and Ewald) when $r < R$.